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The work performed using support from this grant has focused on the following: (1) the development of ZrB2 buffer layers and Si-Ge-Sn compliant templates grown directly upon Si (100), and (2) the demonstration of these systems in mismatched heteroepitaxy of tetrahedral semiconductors including of III-V compounds and group IV materials with Si substrates.

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Final Report

Title: "Synthesis, Characterization, Properties and Performance of Novel Direct Band Gap Semiconductors."

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Summary: The work performed using support from this grant has focused on the following: **(1)** the development of ZrB_2 buffer layers and Si-Ge-Sn compliant templates grown directly upon Si (100), and **(2)** the demonstration of these systems in mismatched heteroepitaxy of tetrahedral semiconductors including of III-V compounds and group IV materials with Si substrates. Highlights of the work are described below:

a) $Ge_{1-y}Sn_y$/Si(100) composite substrates for growth of $In_xGa_{1-x}As$ and $GaAs_{1-x}Sb_x$ alloys:
The growth of III-V semiconductors such as GaAs compounds and $In_xGa_{1-x}As$ and $GaAs_{1-x}Sb_x$ alloys was conducted on Si substrates via lattice-engineered $Ge_{1-y}Sn_y$ buffer layers. These materials are grown directly upon Si(100) strain-free via formation of Lomer edge dislocations at the interface and exhibit a continuous selection of lattice parameters higher than that of Ge allowing close lattice matching with the GaAs, $In_xGa_{1-x}As$ and $GaAs_{1-x}Sb_x$ systems, thereby providing a manifestly different mechanism to the integration of mismatched III-V semiconductors with silicon. As a proof of concept demonstration of the technique a series of $In_xGa_{1-x}As$ and $GaAs_{1-x}Sb_x$ compositions across the entire alloy range were grown using MOCVD at low temperatures between 500-550 °C. The materials displayed high quality morphological, structural and optical properties as evidenced by Rutherford backscattering spectroscopy (RBS), ion channeling, cross sectional transmission electron microscopy (XTEM), atomic force microscopy (AFM), and photoluminescence (PL) characterizations. High resolution x-ray diffraction (XRD) measurements indicated that the films grow with much less strain than those grown on conventional GaAs and III-V bulk substrates.

The applicability of Sn-based buffers on Si to grow technologically relevant ternary III-V alloys represents a straightforward and viable method for large-scale integration. It is more convenient than current state of-the-art multistep methods, involving use of thick $Si_{1-x}Ge_x$ graded layers and chemical mechanical polishing of the layer surface, and produces films of comparable quality. The continuous tunability of the lattice parameter above that of Ge and thermal expansion coefficients within the range of most useful III-V materials, allows films to be grown on Si essentially strain free. In addition to superior microstructure and morphology the facile preparation of the $Ge_{1-y}Sn_y$ buffer layer surface (including surface cleaning and reconstruction) for subsequent heteroepitaxy represents an essential enabling step that further demonstrates the feasibility of these materials as versatile templates for integration of semiconductors with Si.

b) Mismatched heteroepitaxy of tetrahedral semiconductors with Si via ZrB_2 templates:
We have also demonstrated integration of cubic SiC (heterostructures and nanostructures) and assemblies of Ge nanoscale islands with Si substrates via a conductive and reflective ZrB_2 buffer layer. Hexagonal ZrB_2 is grown on cubic Si(111) via a coincidence-misfit mechanism in which the strain is accommodated by edge dislocations along the interface. Ge islands with uniform sizes and strain-free microstructures were grown on ZrB_2/Si(111) at 500 °C via thermolysis of Ge_2H_6, circumventing the strain-driven (Stranski-Krastanov) island formation on Si and

associated limitations. Heteroepitaxy between ZrB_2(0001) and Ge(111) is obtained via alignment of four lattice rows of Ge with every five rows of ZrB_2, (i.e., “magic mismatch”) despite the large difference in lattice constants. Stain-free cubic SiC layers with monocrystalline microstructures and atomically abrupt interfaces are grown on ZrB_2/Si(111) via single source molecular beam epitaxy of $C_2(SiH_3)_2$ at 800 °C. Nanoscale SiC islands with perfectly coherent zinc blende structures are formed at higher temperatures such as 900 °C. The SiC(111)/ZrB_2 interface structures were examined in both cases with high-resolution electron microscopy and compared with optimal bonding configurations derived from theoretical models. A perfect and atomically abrupt interface is observed between the highly planar ZrB_2 surface and the SiC film within the first monolayer of growth.

Publications acknowledging the grant:

1. “Mismatched Heteroepitaxy of Tetrahedral Semiconductors with Si via ZrB_2 Templates”**,** Rahul Trivedi, Po-Liang Liu, Radek Roucka, John Tolle, Andrew V. G. Chizmeshya, Ignatius S. T. Tsong, and John Kouvetakis, Chemistry of Materials, 17, 4647-4652 (2005).
2. “$Ge_{1-y}Sn_y$/Si(100) composite substrates for growth of $In_xGa_{1-x}As$ and $GaAs_{1-x}Sb_x$ alloys”, R. Roucka, J. Tolle, B. Forrest, J. Kouvetakis, V. D'Costa and J. Menendez, Journal of Applied Physics, 101(1), 013518/1-013518/7 (2007).